

# Modeling of Dislocation Structures in Materials

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## Abstract

A phenomenological model of the evolution of an ensemble of interacting dislocations in an isotropic elastic medium is formulated. The line-defect microstructure is described in terms of a spatially coarse-grained order parameter, the dislocation density tensor. The tensor field satisfies a conservation law that derives from the conservation of Burgers vector. Dislocation motion is entirely dissipative and is assumed to be locally driven by the minimization of plastic free energy. We first outline the method and resulting equations of motion to linear order in the dislocation density tensor, obtain various stationary solutions, and give their geometric interpretation. The coupling of the dislocation density to an externally imposed stress field is also addressed, as well as the impact of the field on the stationary solutions.

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## I. INTRODUCTION

The presence and motion of dislocations in materials is known to affect many of their mechanical properties, including, for example, resistance to deformation and plastic response to relatively large stresses [1]. Given the impact of dislocation dynamics on material properties, there have been a number of models advanced attempting to describe the motion of line defects in response to both internal and applied stresses, which have substantially furthered our understanding of these defect-property correlations [2–5].

The starting point of a large class of models of dislocation dynamics is the calculation of direct interactions between a dislocation and a stress field, as given by the Peach-Koehler force [2]. On the one hand it is possible to construct a Newtonian model of dislocation motion by combining the law of conservation of Burgers vector with Newton’s second law, a Hookean stress-strain constitutive law and the differential relation between plastic strain and dislocation density, as has been done elsewhere. [2] While this approach has been very useful in elucidating some important features of dislocation motion, its inherent limitations to relatively short time scales and small numbers of dislocations make its generalization to systems with large numbers of dislocations which evolve over long periods of time somewhat impractical. Numerical calculations of the dynamical evolution of an ensemble of pairwise interacting dislocations have been carried out with Molecular Dynamics methods to study relatively short time scales of the order of several vibrational periods [6]. A different approach to dislocation dynamics is based on purely dissipative or Langevin dynamics [5]. While the level of description is still microscopic, the motion of each dislocation line is assumed to be overdamped. This method allows the study of longer time scales at the price of added phenomenology in the introduction of friction or damping forces.

While the aforementioned approaches have proved quite fruitful, they share several drawbacks that limit their usefulness in studying the evolution of a large ensemble of dislocations over relatively long periods of time. Among them, we note the long ranged nature of dislocation-dislocation interactions which must be truncated in actual calculations, often in

some ad-hoc fashion [4]. In addition, the microscopic nature of the description places a severe restriction to the number of dislocation lines that can be considered. As a consequence, the scale of the resulting microstructure is essentially set by the number of dislocations in a typical simulation cell. We note, however, that recent computational advances have permitted studies involving up to  $10^6$  dislocations [7].

Experimental evidence, on the other hand, suggests that, at least in some cases, the mechanical response of a material may depend only weakly on small-scale microstructural details, and more strongly on the macroscopic density of dislocations. [8] Such evidence implies that an approach based, *a priori*, on the dislocation density might best capture the important macroscopic features of such systems. In this paper we follow this approach and formulate a simplified, linear phenomenological model of dislocation motion, in terms of the dislocation density tensor. The model properly incorporates necessary conservation laws related to the topological structure of the dislocation lines, as well as the true tensorial character of the density. By contrast with previous approaches to this problem, and in the same spirit as irreversible thermodynamics, we employ a non-deterministic description which focuses on a small number of macro-variables and treats the remaining degrees of freedom, which are presumed to evolve on a faster time scale, as an effective heat bath. This is formally accomplished by applying a coarse-graining procedure to a system of dislocations in an elastically isotropic medium, and selecting the dislocation density tensor as the appropriate order parameter to describe the system at this scale. Of course, this approach is formally equivalent to Langevin type models mentioned earlier: dislocation motion is overdamped because of its interaction with other microscopic degrees of freedom that act as a “heat bath”. We argue, however, that the overdamped character of dislocation motion arises only at a semi-macroscopic scale, and that it includes not only interactions with the “heat bath”, but also mutual dislocation interactions within a coarse-graining cell.

Our approach also parallels the study of the equilibrium statistical mechanics of a system of unbound dislocations undertaken by Nelson and Toner [9]. They investigated the effect of a collection of dislocations on the broken translational and rotational symmetries of

the crystalline state by examining the Fourier transform of the dislocation density-density correlation function at long wavelengths. In so doing, they argued that dislocations destroy long-ranged translational order, but not long-ranged orientational order. [9] Central to this calculation is the identification of the appropriate Boltzmann weight (and therefore the free energy) that determines the probability of the occurrence of a given fluctuation, and of the corresponding defect configuration. In their view the relevant dislocation driving forces can be constructed from a free energy which is a functional of the dislocation density tensor, with components  $\rho_{ij}$ , and a non-singular strain, with components  $e_{ij}^{NS}$ , which describes vibrational degrees of freedom in the crystal. The contribution to the free energy that depends on  $\rho_{ij}$  was chosen equal to the energy of interaction between dislocations, as derived by Kosevich [10]. The logical next step, which we propose here, is to use the minimization of the singular contribution to the free energy as the driving force for dislocation motion.

We finally mention complementary earlier work by Brand and Kawasaki [11–13], who derived phase equations for generic systems that support topological defects. A phase equation involves a phase variable that changes slowly on the scale of the lattice spacing and in time, and that has a nonzero winding number around a topological defect. This type of equation represents the long-wavelength distortion of some ideal basic pattern and has been successfully used in a large variety of nonequilibrium systems [14]. We focus our attention on the case of a crystalline solid and retain the full dislocation density tensor in our description, since we believe that this is the natural coarse-grained variable to describe a defected crystalline solid. Our choice of variables may prove useful in two different directions. First, the equations that we present below may provide a starting point for direct numerical calculations of dislocation motion, a subject of considerable interest. Second, coupling to other slow variables of interest can be accomplished quite naturally. These would include, for example, energy or mass densities. The latter are necessary to describe other irreversible phenomena such as the effect of mass diffusion on dislocation motion.

This paper is organized as follows. In Sec. II we describe the dynamical equations governing the evolution of the dislocation density in an isotropic elastic medium. In Sec.

III stationary solutions are identified and given geometrical interpretations, both in systems with and without externally imposed stresses. Finally, Sec. IV contains a short summary and discussion of future work.

## II. MODEL EQUATIONS

Consider an isothermal, three-dimensional, linear isotropic elastic medium which contains a large, finite number of unbound dislocation lines which are free to move throughout the system. Suppose further that this medium is subdivided into a number of hypothetical averaging cells, each of volume  $V_0$ , such that a relatively large number of dislocation lines thread a given volume element. Now, if one wishes to describe the defect properties of this system on a length scale larger than  $(V_0)^{1/3}$ , then one can define a coarse-grained variable, the dislocation density, which reflects the average dislocation content of a cell. As a dislocation is characterized by two directions in space, its line direction,  $\hat{\chi}$ , and the direction of its Burgers vector,  $\vec{b}$ , it is expected that the dislocation density must also carry such information and would, therefore, be a second-rank tensor. The components of this tensor will be denoted by  $\rho_{ij}$  hereafter.

In modeling the dynamics of the defected system described above at this coarse-grained level, it is necessary to include “slow” variables, the relaxation of which takes place on time scales much longer than microscopic times [15,16]. Variables that satisfy global conservation laws or that arise as a consequence of a spontaneously broken symmetry satisfy this requirement. Although line defects are not present in equilibrium in a three dimensional crystalline solid, we take the view that there exists a time scale, slow compared to relevant experimental times, in which the net Burgers vector in a crystalline solid is conserved. In practice, of course, dislocations may migrate to the surface of the crystal or to a grain boundary and disappear. Conservation of Burgers vector can be expressed in terms of the dislocation density tensor  $\rho_{ij}$  as [10]

$$\frac{\partial \rho_{ij}}{\partial t} + \epsilon_{ilm} \frac{\partial j_{mj}}{\partial x_l} = 0, \quad (1)$$

where  $\epsilon_{ilm}$  are the components of the Levi-Civita tensor density,  $j_{mj}$  are the components of a dislocation flux density tensor which govern the flow of Burgers vector in the medium and we have adopted the convention that repeated indices are summed over. The dislocation density tensor satisfies the relation,

$$\int \rho_{ij} dS_i = b_j, \quad (2)$$

where the integral extends over an arbitrary surface in the crystal, and  $b_j$  is the  $j$ -component of the sum of Burgers vectors of all the dislocation lines that cross the surface. It should also be noted here that the subsidiary constraint

$$\frac{\partial \rho_{ij}}{\partial x_i} = 0 \quad (3)$$

that the dislocation density be solenoidal must also be imposed to ensure that dislocation lines do not terminate within the solid, except perhaps at some internal interface such as a grain boundary. The necessity of incorporating this requirement was demonstrated by Nabarro. [17]

Equation (1) is correct microscopically, but involves the unknown flux  $j_{mj}$ , now a second rank tensor. We note that this equation has already been used as the starting point in other theories of dislocation dynamics [18,3] and that our approach differs in our choice of the flux  $j_{mj}$ . As discussed earlier, expressions for the flux are derived invoking the Peach-Koehler force and continuum elasticity, and therefore yield equations that are invariant under time reversal. We suggest instead that dislocation motion is overdamped at the coarse-grained scale of motion, and that a constitutive equation for the flux can be introduced such that the dislocation density tensor evolves to minimize the local free energy of the defected material. The origin of this dissipative motion lies both in interactions with other microscopic degrees of freedom and interactions with other dislocations within the coarse-graining cell. As a consequence, our equations are manifestly not invariant under time reversal.

As described earlier, the free energy of the crystal is a functional of the dislocation density tensor, and a non-singular strain  $e_{ij}^{NS}$ , which describes phonon modes. It is useful to regard

these two tensor fields as part of the basis of an abstract Hilbert space of slow variables which characterizes the system. Further, if these two fields are mutually orthogonal then, following Nelson and Toner [9],

$$F = F_{NS} [e_{ij}^{NS}] + F_d [\rho_{ij}], \quad (4)$$

where  $F_{NS}$  and  $F_d$  are the non-singular and the dislocation parts of the free energy, respectively.

The spontaneous evolution of the system from some initial dislocation configuration towards equilibrium results in a decrease in its free energy (at constant temperature). We neglect in what follows the nonsingular contribution to free energy dissipation since for the phenomena of interest the associated time scale for phonon propagation is expected to be much shorter than that for dislocation motion. With this in mind, we have that the time rate of change of the free energy is given by

$$\frac{dF}{dt} = \int d^3r \left( \frac{\delta F_d}{\delta \rho_{ij}} \right) \left( \frac{\partial \rho_{ij}}{\partial t} \right), \quad (5)$$

where  $\delta/\delta \rho_{ij}$  stands for functional or variational derivative with respect to  $\rho_{ij}$ , the integral extends over the entire system, and we have chosen appropriate boundary conditions so that surface integrals vanish. Upon substituting the conservation law (Eq. (1)) and integrating by parts, the requirements that the total free energy be a monotonically decreasing function of time, and that there be a linear relation between forces and fluxes, leads to the identification of the dissipative dislocation density flux,

$$j_{mj} = -B_{mjst} \epsilon_{sab} \frac{\partial}{\partial x_b} \left( \frac{\delta F_D}{\delta \rho_{at}} \right), \quad (6)$$

where the fourth-rank tensor,  $B_{mjst}$  plays the role of kinetic or Onsager coefficient, and embodies the complicated microscopic dynamics that allows the reduction in free energy at the coarse-grained scale. Substitution of Eq. (6) into the conservation law, Eq. (1), leads to the dynamical equation for the dislocation density tensor.

Further simplification is possible when the kinetic attributes of the medium under consideration are spatially isotropic. In this case the Curie principle [19] constrains the form of the tensor of kinetic coefficients to

$$B_{mjst} = \bar{B} \left[ \frac{1}{2} (\delta_{mt}\delta_{js} + \delta_{ms}\delta_{jt}) - \frac{1}{3}\delta_{mj}\delta_{st} \right], \quad (7)$$

where  $\bar{B}$  is the single required kinetic coefficient. It is also possible to modify this description in order to distinguish between glide and climb kinetics, though we will leave this modification for later work. As our formulation focuses on the coarse-grained dislocation density, the phenomenological constant  $\bar{B}$  can only provide limited insight into the details of the mechanism for defect motion since, for example, the detailed geometry of slip planes and directions has been averaged over. Nevertheless, as will be shown below, one can extract interesting microstructural information from our model, and so there is an implicit information trade-off in this approach to the problem.

The only quantity that remains to be specified is the free energy density corresponding to the singular part of the deformation field, and to express it explicitly as a function of the dislocation density tensor. Kosevich [10] has already calculated the elastic energy of interaction between sets of dislocations, and this result was later adopted by Nelson and Toner [9] for equilibrium calculations [20]. The result is most conveniently expressed in terms of an integration in reciprocal space by

$$F_d = \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} K_{ijkl}(\vec{q}) \rho_{ij}(\vec{q}) \rho_{kl}(-\vec{q}) \quad (8)$$

with

$$K_{ijkl}(\vec{q}) = K_{ijkl}^0(\vec{q}) + K_{ijkl}^c(\vec{q}), \quad (9)$$

where the main kernel  $K_{ijkl}^0$  is given in terms of the shear modulus  $\mu$  and Poisson ration  $\nu$  by

$$K_{ijkl}^0(\vec{q}) = \frac{\mu}{q^2} \left[ Q_{ik}Q_{jl} + C_{il}C_{kj} + \frac{2\nu}{1-\nu}C_{ij}C_{kl} \right] \quad (10)$$



and the core kernel  $K_{ijkl}^c$  is given in terms of the edge and screw core energies (per unit length),  $E_e$  and  $E_s$ , by

$$K_{ijkl}^c(\vec{q}) = 2E_e\delta_{ik}\delta_{jl} + 2(E_s - E_e)\delta_{ij}\delta_{kl}. \quad (11)$$

It is advantageous to express these kernels in terms of the transverse and rotational  $\vec{q}$ -space projection operators

$$Q_{ij} = \delta_{ij} - \frac{q_i q_j}{q^2}, \quad (12)$$

$$C_{ij} = \epsilon_{ijl} \frac{q_l}{q}, \quad (13)$$

respectively, as will be evident below.

Before we proceed any further, we point out here that, upon substituting the densities corresponding to single isolated dislocations into Eq. (8), one recovers the familiar Peach-Koehler interaction [2]. For example, consider two infinite, parallel screw dislocations, with Burgers vectors  $\vec{b}^{(1)}$  and  $\vec{b}^{(2)}$ , which are located at the origin and at  $\vec{a}$ , respectively. The Fourier transforms of the dislocation densities corresponding to these defects are then

$$\rho_{ij}^{(1)}(\vec{q}) = 2\pi b^{(1)} \delta_{i3} \delta_{j3} \delta(q_z), \quad (14)$$

$$\rho_{ij}^{(2)}(\vec{q}) = 2\pi b^{(2)} \delta_{i3} \delta_{j3} \delta(q_z) e^{-i\vec{q}\cdot\vec{a}} \quad (15)$$

and the line direction is along the  $z$ -axis. Neglecting the core contributions for the moment, one finds that the interaction free energy per unit dislocation length is

$$-\frac{\mu b^{(1)} b^{(2)}}{2\pi^2} \int d^2 q \frac{1}{q^2} e^{-i\vec{q}\cdot\vec{a}} = -\frac{\mu}{2\pi} b^{(1)} b^{(2)} \ln(a), \quad (16)$$

implying that the associated force (per unit length)  $= \mu b^{(1)} b^{(2)} / 2\pi a$ , as expected. Thus, the main kernel given by Eq. (10) embodies long-ranged interactions among dislocations.

The effect of an external stress field with components  $\sigma_{ij}^0$  on a collection of dislocations can also be incorporated by the addition to the free energy  $F_d$ , of a term representing the interaction of the dislocation density with the external field. Following Mura [6], we write  $F_{ext}$  as

$$F_{ext} = - \int d^3r \sigma_{ij}^0 \epsilon_{ij}^*, \quad (17)$$

where  $\epsilon_{ij}^*$  is the eigenstrain associated with a particular dislocation density tensor configuration, and the total free energy is then  $F_{tot} = F_d + F_{ext}$ . We will elaborate further on this issue below.

By combining the results summarized above, one finally arrives at the equation of motion for the dislocation density tensor,

$$\frac{\partial \rho_{ij}(\vec{q})}{\partial t} = q^2 C_{mi} C_{sa} B_{mjst} \frac{\delta F_{tot}}{\delta \rho_{at}(-\vec{q})}. \quad (18)$$

### III. STATIONARY SOLUTIONS

Clearly, equation (18) is linear in the dislocation density tensor and will therefore only describe the linear relaxation of a defected system towards the asymptotic state of thermodynamic equilibrium, given by the minimization of  $F_{tot}$ . The relaxation rate as a function of wavevector  $\vec{q}$  can be directly obtained from the eigenvalues of the kernel of Eq. (18).

It is of interest to first study those eigenmodes of zero eigenvalue; i.e., the stationary solutions. We start by examining the equilibrium solutions, i.e., configurations of defects that minimize the free energy.

#### A. Equilibrium configuration without external stress

We first consider the free energy  $F_d$  in the absence of external stresses and seek those densities that satisfy

$$\frac{\delta F_d}{\delta \rho_{at}(-\vec{q})} = [K_{atpq}^0(\vec{q}) + K_{atpq}^c(\vec{q})] \rho_{pq}(\vec{q}) = 0. \quad (19)$$

The kernel can be regarded as a 9x9 Voigt matrix with components  $K_{\alpha\beta}$  ( $1 \leq \alpha, \beta \leq 9$ ) and, since  $K_{\alpha\beta} = K_{\beta\alpha}$ , its eigenvalue spectrum is real. This kernel is non-singular and therefore the only eigenstates with zero eigenvalue are the trivial ones:  $\rho_{pq} = 0$ , i.e., a

defect free medium. This fact immediately follows from the core contribution to the free energy (Eq. (11)). However, Eq. (19) also supports defected equilibrium states for a system constrained to having nonzero densities  $\rho_{pq}$ . The Lagrange multipliers for such a constrained minimization can be chosen so as to cancel the core contribution, so that the problem therefore reduces to finding the (non-trivial) eigenstates of the kernel  $K_{atpq}^0$  which have zero eigenvalue. This latter kernel is singular, hence one expects that there will be at least one such zero eigenstate.

For this purpose it is convenient to express the dislocation density in terms of the operators which comprise the main kernel. For a rotationally invariant system one can form three second-rank tensors from  $\vec{q}$ :  $\delta_{ij}$ ,  $q_i q_j$  and  $\epsilon_{ijk} q_k$ . We therefore use the decomposition [16]

$$\rho_{ij}(\vec{q}) = \delta_{ij}X(q) + P_{ij}Y(q) + C_{ij}Z(q), \quad (20)$$

where the longitudinal projector  $P_{ij} = \delta_{ij} - Q_{ij}$ , and where  $X$ ,  $Y$  and  $Z$  are three  $q$ -dependent amplitudes. Such a decomposition has the advantage that it permits the classification of the density in terms of its parity since, for example,  $P_{ij}$  and  $C_{ij}$  have different signatures under parity. Also, it is possible to determine the edge and screw character of the density by noting that for an edge (screw) dislocation the Burgers vector  $\vec{b}$  is perpendicular (parallel or anti-parallel) to its line direction. Hence,  $\rho_{ij}$  is of edge (screw) character if  $\rho_{ij} \neq 0$  for  $i \neq j$  ( $i = j$ ). The effect of the main kernel on the dislocation density can then be determined from the results of the operator algebra summarized below:

$$C_{sa}C_{aq} = -Q_{sq} \quad (21)$$

$$C_{sa}Q_{ap} = C_{sp} = Q_{sa}C_{ap} \quad (22)$$

$$Q_{ia}Q_{ab} = Q_{ib} \quad (23)$$

With the preceding relations in mind, one can immediately identify several degenerate eigenstates with zero eigenvalue by observing that

$$K_{atpq}^0 Q_{pq} = 0, \quad (24)$$

$$K_{atpq}^0 \delta_{pq} = 0, \quad (25)$$

and, consequently,  $P_{pq}$  is also an eigenstate. For the problem under consideration, then,  $Q_{pq}$  is an acceptable eigenstate as it is solenoidal while  $\delta_{pq}$  clearly does not satisfy this requirement. In the former case, the transverse operator can be represented in real space by performing an inverse Fourier transformation to obtain

$$Q_{pq}(\vec{r}) = \frac{1}{(2\pi)^3} \left[ \left( \frac{1}{r^3} \delta_{pq} - \frac{3x_p x_q}{r^5} \right) + 2\delta(\vec{r}) \delta_{pq} \right] \quad (26)$$

Thus, the dislocation density falls off like  $1/r^3$  and has a quadrupolar angular dependence.

There are other degenerate eigenstates which correspond to more spatially localized dislocation densities and that break rotational invariance. As an example, consider the line along  $q_1$  in reciprocal space

$$\rho_{pq} = A [\delta_{pq} - \delta_{p1} \delta_{q1}] \delta(\vec{q}_2) \delta(\vec{q}_3), \quad (27)$$

which is an eigenstate of the main kernel with zero eigenvalue, given that  $A$  is a dimensional constant that is independent of wavevector. This particular combination of delta functions was chosen to ensure that the density is solenoidal. Now, this line in reciprocal space maps into the  $x_2 - x_3$  plane in real space. Further, the fact that the only two non-zero components are  $\rho_{22}$  and  $\rho_{33}$  implies that the density has screw character. In short, Eq. (27) corresponds to a two-dimensional dislocation “wall” in real space. The screw character of the wall implies that it can be regarded, in some sense, as a prototypical (low-angle) twist grain boundary. It is interesting to note that such a regular distribution of dislocations might be expected from the tendency of dislocations to polygonize. In this model, however, such a structure has been obtained without postulating the existence of additional “chemical” forces, related to vacancy concentration at dislocations, which inhibit climb. Walls of other orientations are, of course, also possible.

## B. With External Stress

In many cases of interest the defected system will be subjected to an externally imposed stress field. Equation (18) also applies in this case, with the free energy explicitly including the contribution arising from the imposed stress. Now, in order to apply our previous results, it is first necessary to relate the eigenstrain in Eq. (17) to the dislocation density. Such a relation may be constructed by noting that the eigenstrains for this problem arise from plastic distortion, and that the essential connection between plastic strain and the Burgers vector of a dislocation can be expressed in terms of the closure failure of a Burgers circuit that encircles the dislocation. Generalizing this idea to a collection of dislocations leads to

$$\rho_{ij}(\vec{r}) = -\epsilon_{ilm} \frac{\partial \beta_{mj}^P}{\partial x_l}, \quad (28)$$

where the components of the plastic distortion tensor  $\beta_{ij}^P$  are related to the eigenstrain by  $\epsilon_{ij}^* = (1/2)(\beta_{ij}^P + \beta_{ji}^P)$ . It should be noted here that Eq. (28) by itself does not uniquely define the plastic strain. In particular, it does not specify the divergence of the plastic strain and so some additional input, such as the specification of a gauge, is required. The role of gauge invariance in the field theory of dislocations has been discussed elsewhere. [21]. In the present context this additional input is contained implicitly in Eq. (6) since the dislocation flux is related to the time-rate change of the plastic distortion by  $j_{mk} = -\partial \epsilon_{mk}^* / \partial t$ , a relation indicated by Kroner and Rieder [22]. Further, from the form on the kinetic coefficient employed in Eq. (6), it is evident that  $j_{mm} = 0$ , and so there is no time rate change of the volume associated with plastic deformation.

With this in mind, we consider here, for the purpose of illustration, the specific case of a symmetric, solenoidal external stress tensor given in reciprocal space by

$$\sigma_{ij}^0(\vec{q}) = \bar{\sigma}(q) Q_{ij}, \quad (29)$$

where  $\bar{\sigma}(q)$  is a function of the wavenumber  $q$ . For this case  $F_{ext}$  becomes

$$F_{ext} = - \int \frac{d^3 q}{2\pi^3} \bar{\sigma}(q) Q_{ij} \epsilon_{ij}^*(-\vec{q}) = i \int \frac{d^3 q}{2\pi^3} \frac{\bar{\sigma}(q)}{q} C_{ij} \rho_{ij}(-\vec{q}), \quad (30)$$

where Eq. (28) has been used to relate the transverse projection of the dislocation density to the rotational projection. So, the state of equilibrium is defined by the eigenvalue equation

$$\frac{\delta F_{tot}}{\delta \rho_{at}(-\vec{q})} = K_{atpq}^0(\vec{q})\rho_{pq}(\vec{q}) + \frac{i}{q}\bar{\sigma}C_{at} = 0. \quad (31)$$

A solution to this eigenvalue problem can be obtained by noting that  $C_{ij}$  itself is an eigenstate of the main kernel since

$$K_{ijkl}^0 C_{kl} = 2\frac{1+\nu}{1-\nu}C_{ij}, \quad (32)$$

and so an equilibrium configuration (in reciprocal space) is given by

$$\rho_{pq}(\vec{q}) = \frac{-i}{2q}C_{pq}\bar{\sigma}(q)\frac{1-\nu}{1+\nu}, \quad (33)$$

or in real space by

$$\rho_{pq}(\vec{r}) = \int d^3r' \bar{\sigma}(\vec{r}') L_{pq}(\vec{r} - \vec{r}'), \quad (34)$$

where

$$L_{pq}(\vec{r}) = \frac{-1}{8\pi} \frac{1-\nu}{1+\nu} \frac{\epsilon_{pql}x_l}{r^3}. \quad (35)$$

Thus, the application of a “transverse” stress field results in a dislocation density with “rotational” character.

Since, as indicated above, Eq. (6) relates the time-rate change of the eigenstrain to the dislocation density, it is advisable in the case of an arbitrary (symmetric) external stress to first develop an equation for the temporal evolution of the Fourier transform of the eigenstrain,  $\epsilon_{ij}^*(\vec{q})$ , and then determine the dislocation density by using the Fourier transform of Eq. (28)

$$\rho_{ij}(\vec{q}) = -iqC_{im}\beta_{mj}^P. \quad (36)$$

or the symmetrized form

$$q^2 \epsilon_{ilm}\epsilon_{jpk} P_{lp}\epsilon_{mk}^* = \eta_{ij}, \quad (37)$$

where  $\eta_{ij}$  is Kroner's incompatibility tensor [23], which is essentially the Ricci tensor and therefore a measure of curvature. [24] Such an equation can be determined by using Equations (6), (10), (19) and (17) to obtain

$$\frac{\partial \epsilon_{mk}^*}{\partial t} = \mu B_{mkst} \left[ Q_{sq} Q_{tp} + Q_{sp} Q_{tq} - \frac{2\nu}{1-\nu} Q_{st} Q_{pq} - \sigma_{pq}^0 \right] \epsilon_{pq}^*. \quad (38)$$

Thus, both the dislocation density and the eigenstrain can be determined from this formulation. Further, since the dependence of the eigenstrain on time is dependent on the dislocation flux, the value of the eigenstrain will depend upon the time history of the system, as expected.

Equations (36) and (38) can be used to identify the dislocation density corresponding to a specific plastic strain. For example, in the case of no externally applied stress field, the plastic distortion  $\beta_{ij}^P = P_{ij}$  corresponds to  $\rho_{ij} = 0$ , whereas the plastic distortion  $\beta_{ij}^P = C_{ij}$  (and therefore  $\epsilon_{ij}^P = 0$ ) corresponds to  $\rho_{ij} = Q_{ij}$ . In each case, the plastic strain and the corresponding dislocation density of these equilibrium states are time-independent.

Finally we address the issue of whether there exist other stationary solutions of the dynamic equations that are not minima of the free energy. We show next that the tensor  $C_{mi} C_{sa} B_{mjst}$ , the generalized kinetic coefficient in Eq. (18), commutes with the linear kernel  $K^0$  for the class of solutions that do not break rotational invariance. Hence all the stationary solutions of the dynamics are minima of the free energy. Given the general decomposition for a rotationally invariant system of Eq. (20), and the fact that  $\delta_{ij}$ ,  $Q_{ij}$  and  $C_{ij}$  are eigenstates of  $K^0$ , it is sufficient to show that  $\delta_{ij}$ ,  $Q_{ij}$  and  $C_{ij}$  are also eigenstates of  $C_{mi} C_{sa} B_{mjst}$ .

First, by using Eqs. (7) and (22), we find

$$C_{mi} C_{sa} B_{mjst} Q_{at} = \bar{B} C_{mi} \left[ \frac{1}{2} (C_{jm} + C_{mj}) - \frac{1}{3} \delta_{mj} C_{ss} \right] = 0. \quad (39)$$

The first term vanishes because  $C_{ij}$  is an antisymmetric tensor. The second vanishes because  $C_{ij}$  is proportional to the Levi-Civita tensor. Similarly, by using Eqs. (7), (21) and (22) we find

$$C_{mi} C_{sa} B_{mjst} C_{at} = -\bar{B} C_{mi} \left[ \frac{1}{2} (Q_{mj} + Q_{jm}) - \frac{1}{3} \delta_{mj} Q_{ss} \right] = \bar{B} \left( -C_{ij} + \frac{2}{3} C_{ij} \right), \quad (40)$$

where we have used the fact that  $Q_{ij}$  is symmetric and that  $Q_{ss} = 2$ . Finally,

$$C_{mi}C_{sa}B_{mjst}\delta_{at} = \bar{B}C_{mi}\left[\frac{1}{2}(C_{mj} + C_{jm}) - \frac{1}{3}\delta_{mj}\delta_{ts}C_{st}\right] = 0. \quad (41)$$

#### IV. CONCLUSIONS

We have considered a formal coarse-graining procedure over elements of volume that contain a large number of dislocation lines, and argued that microscopic interactions among the lines within each element of volume give rise to dissipative macroscopic dynamics. A constitutive law relating the dislocation density tensor and its associated flux has been introduced such that the evolution of the defected system is driven by the minimization of its plastic free energy. A standard procedure based on linear irreversible thermodynamics leads to the equations of motion for the dislocation density.

For the case of an isotropic medium, the energy of interaction between dislocations in terms of the dislocation density tensor had already been calculated by Kosevich. We have further shown that in this case the tensor of kinetic coefficients that appears in the kinetic law requires only the specification of a scalar quantity, and that it commutes with the kernel of the linear operator driving energy minimization. Some stationary solutions have been explicitly constructed, both in systems with and without externally imposed stresses.

We have restricted our attention in this paper to idealized systems wherein there is no mechanism for dislocation production, such as a Frank-Read source. [2] It is possible, however, to incorporate a stochastic “source” term in Eq. (6) satisfying a fluctuation-dissipation relation to model dislocation production. This would be useful in examining, for example, the change in mechanical properties that attend dislocation formation, such as work hardening.

Finally, given that the approach discussed here is based on having partially averaged microscopic degrees of freedom, it seems of interest to relate it to results from microscopic descriptions such as the ones outlined in the Introduction. For example, one might consider



the dynamical evolution that results from these other models and then invoke a coarse-graining procedure. This, of course, would require systems that contain a large number of dislocations and, as mentioned above, algorithms for such large systems have or are currently being developed. Thus, it may be possible to bridge the disparate length scales between both descriptions.

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